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The Liquid Structure of the N-Paraffins

A. B. Carr
State University of Iowa

has sometimes been questioned whether the laboratory does act effectively either as inspiration or as a teaching device. The paper describes experiences in a laboratory where the experiments were exactly correlated with the class work, where laboratory manual was dispensed with, where the experiments were usually unconventional.

DEPARTMENT OF PHYSICS,
STATE UNIVERSITY OF IOWA,
IOWA CITY, IOWA.

THE LIQUID STRUCTURE OF THE N-PARAFFINS.

A. B. CARR

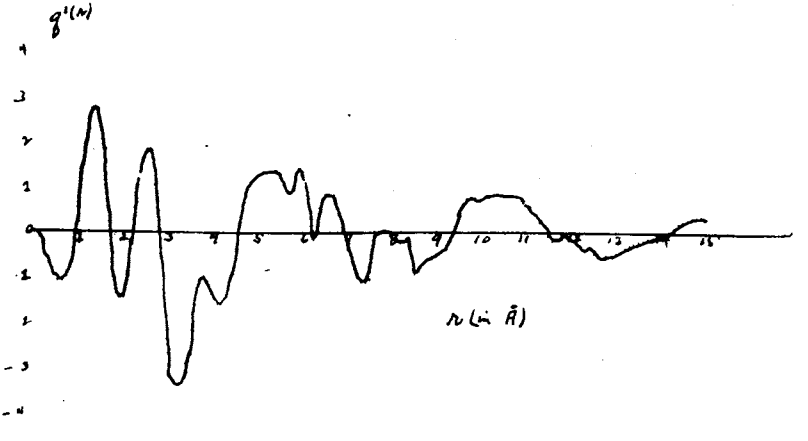
The object of this investigation is to determine whether or not Pierce's density computations compare the more favorably with the hexagonal or the square array.

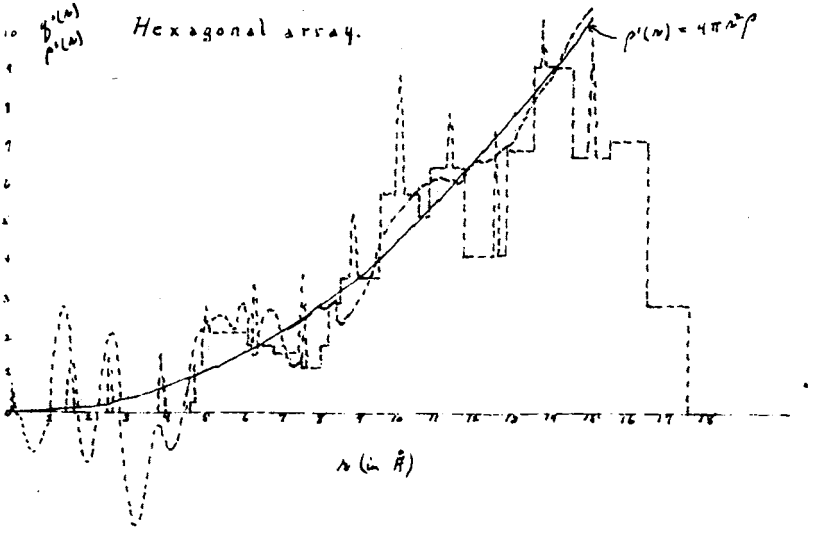
Professor W. C. Pierce, Department of Chemistry, University of Chicago, in an article in the Journal of Chemical Physics, Vol. 3, pp. 252-255, on Scattering of X-rays by Polyatomic Liquids. n-Heptane says "recent publications in the field of x-ray scattering by liquids have led the writer to the questions:

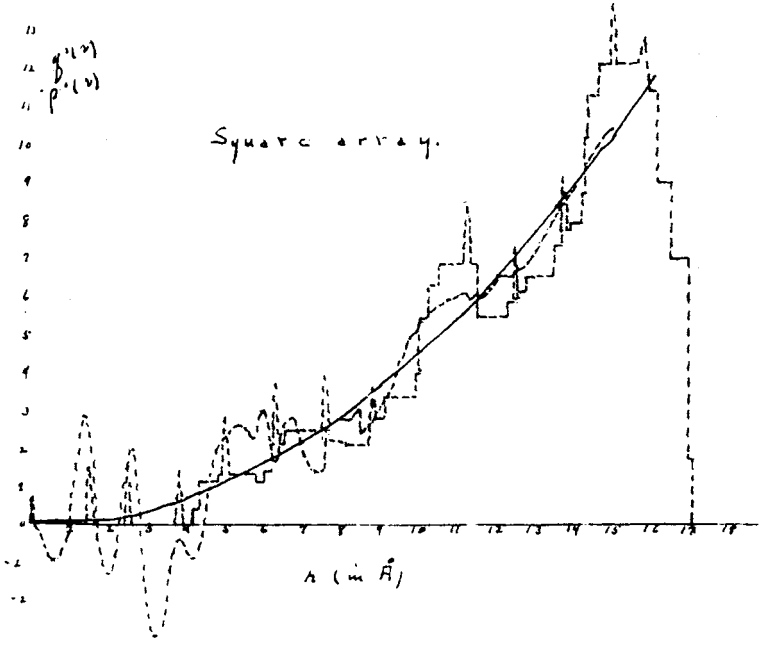
(a) How much information concerning the structure of single molecules may be obtained from liquids scattering data?

(b) Is the use of the Fourier integral theorem valid for data extending over a small range of sin ϑ/λ?

These computations are concerned with the first question mostly. The number of atoms and their computed distance, (r), from the reference atom were determined for the hexagonal and the square




Hexagonal array.
$\rho'(r) = 4\pi r^2 \rho$
r (in Å)


Square array.
r (in Å)

array. In the central molecule, the distance, (r), was determined as from the reference atom to the actual positions of the atoms in the molecule. To compute the distance from the selected atom to the atoms in a neighboring molecule, the selected atom and the atoms in the neighboring molecule are considered as being on the axis of rotation of the molecule. The distance (r) in both arrays were computed for a maximum distance of 16 Angstroms.

Now plot the number of atoms, $\varrho^1(r)$, as ordinates against distances, (r) in Angstroms, as abscissa, using blocks. All adjacent molecules are spread over 0.1 A., all in the same molecule triangles are used, 0.25 A. The unit area is 0.1 A by 1 unit of (r).

Since the area under the curve is $\int 4\pi r^2 \varrho .\, dr$ which corresponds to $\int y\, dx$, y is $4\pi r^2 \varrho$. This gives ordinates, y, values for the final curve, $\varrho^1(r)$.

Having obtained the $\varrho^1(r)$ curve, Pierce's curve was plotted upon it using the $\varrho^1(r)$ curve as an axis.

Slide 1 shows Pierce's distribution function for n-heptane. The $q^1(r)$ values give the number of atoms in excess of the average at radial distance, (r).

Slide 2 shows Pierce's curve on my curve for the hexagonal array. There is fair agreement for (r) in the region 4.5 to 7 A. From 8.5 to 9.5 A and from 11.7 to 16 A the comparison is poor.

Slide 3 shows Pierce's curve on my curve for the square array. From (r) 7 to 12 A there is good agreement while from about 4 to 6.5 A agreement is bad.

The conclusion is reached that no certain discrimination can be made with present methods.

Simpson College,
Indianola,
State University of Iowa,
Iowa City, Iowa.